

Anderson tower of states and nematic order of spin-1 bosonic atoms on a 2D lattice

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We investigate the structure of the spectrum of antiferromagnetically coupled spin-1 bosons on a square lattice using degenerate perturbation theory and exact diagonalizations of finite clusters. We show that the superfluid phase develops an Anderson tower of states typical of nematic long-range order with broken $SU(2)$ symmetry. We further show that this order persists into the Mott insulating phase down to zero hopping for one boson per site, and down to a critical hopping for two bosons per site, in agreement with mean-field and Quantum Monte Carlo results. The connection with the transition between a fragmented condensate and a polar one in a single trap is briefly discussed.

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INTRODUCTION

Spinor Bose gases have been the subject of a very intensive activity over the past fifteen years, both experimentally and theoretically [1–4]. For spin-1 bosons, the spin-spin interaction can be ferromagnetic or antiferromagnetic depending on the relative scattering lengths in the $S = 0$ and $S = 2$ channels, leading in a harmonic trap to a ferromagnetic or to a singlet condensate [5, 6]. When an optical lattice is introduced, the system can in addition turn into a Mott insulator at commensurate filling if the tunneling amplitude is small enough as compared to the on-site repulsion. In the single-band approximation at each site, such systems can be described by the Bose-Hubbard Hamiltonian [7, 8]:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} (a_{i,\sigma}^\dagger a_{j,\sigma} + \text{H.c.}) + \frac{U_0}{2} \sum_i n_i(n_i - 1) + \frac{U_2}{2} \sum_i (\vec{S}_i^2 - 2n_i) \quad (1)$$

where $\langle i, j \rangle$ stands for pairs of nearest neighbors, $\sigma = -1, 0, 1$ is the spin, $a_{i,\sigma}^\dagger$ and $a_{i,\sigma}$ are creation and annihilation operators of spin-1 bosons at site i , while $n_i = \sum_\sigma n_{\sigma i} = \sum_\sigma a_{\sigma i}^\dagger a_{\sigma i}$ and \vec{S}_i are the density and spin operators at site i . The parameters of this model are the tunneling amplitude $t > 0$, the on-site repulsion $U_0 > 0$, and the on-site spin-spin interaction U_2 , which is positive (negative) for antiferromagnetic (ferromagnetic) interactions.

The mean-field phase diagram of the antiferromagnetic version of the model has been mapped out quite some time ago by A. Imambekov *et al.* [8], who found that the odd-density Mott insulating phases are completely nematic while the even-density ones undergo a transition from a non-magnetic singlet phase to a nematic phase upon increasing the ratio t/U_0 . In view of the competing orders (such as valence-bond solid order reported in 1D [9–11]), this result clearly calls for further investigations beyond mean-field. The first attempt has been done recently using Quantum Monte Carlo, which has no minus sign problem for this type of bosonic Hamiltonian [12]. This investigation revealed the presence of a local quadrupolar

moment in the entire Mott insulating phase with one boson per site, while a local quadrupolar moment only develops for large enough hopping in the Mott insulating phase with two bosons per site. This is consistent with the mean-field phase diagram, but one should keep in mind that the numerical demonstration of nematic long-range order would require an investigation of quadrupolar correlations, which was beyond the scope of Ref. [12]. So further work is definitely needed to check the presence of nematic long-range order in the phase diagram of the model of Eq. 1.

In this Letter, we show that the superfluid phase of spin-1 bosons with antiferromagnetic interactions indeed develops true nematic long-range order in the presence of a lattice. This conclusion is based on a careful investigation of the excitation spectrum of the model using degenerate perturbation theory in the limit $U_0 = 0, U_2/t \rightarrow 0$ and exact diagonalizations of finite clusters away from that limit. The key observation is that, in the presence of a lattice, the spectrum acquires the structure of an Anderson tower of states, *i.e.* a family of low-lying states whose energy collapses onto that of the ground state in the thermodynamic limit, and that all these states have even values of the total spin, so that polar states (and not antiferromagnetic states) can be reconstructed as linear combinations of degenerate ground states. Exact diagonalizations are further used to show that this structure persists in the Mott insulating phase as long as nematic order is present, leading to an alternative determination of the singlet-nematic transition in the $S = 2$ Mott insulator.

Let us start by solving the problem analytically in the limit $U_0 = 0, U_2/t \rightarrow 0$ which, as we shall show later, turns out to be representative of the general case. Let us denote by N_s the number of sites and by N the number of bosons. In the non-interacting case ($U_0 = U_2 = 0$), the bosons condense in the $\vec{k} = \vec{0}$ state, but since there is no magnetic interaction, the spin is irrelevant, and the ground state is vastly degenerate. The ground states are given by

$$|\psi_{n_{-1}, n_0, n_1}\rangle = \prod_\sigma \frac{a_{\vec{k}=\vec{0}, \sigma}^{\dagger n_\sigma}}{\sqrt{n_\sigma!}} |0\rangle \quad (2)$$

with $\sum_{\sigma} n_{\sigma} = N$ and $a_{\vec{k}=\vec{0},\sigma}^{\dagger} = (1/\sqrt{N_s}) \sum_{i=1}^{N_s} a_{i,\sigma}^{\dagger}$. The degeneracy is equal to $(N+1)(N+2)/2$.

Let us now consider the effect of U_2 . If U_2/t is small, we can use degenerate perturbation theory, which means that we must diagonalize $\sum_i \vec{S}_i^2$ in the subspace spanned by the degenerate ground states of Eq.(2). Now, this operator commutes with the square of the total spin $\vec{S}_{\text{tot}} = \sum_i \vec{S}_i$. So, in the basis of the eigenstates of \vec{S}_{tot}^2 , the matrix of $\sum_i \vec{S}_i^2$ is diagonal, and the problem reduces to the evaluation of the expectation value of $\sum_i \vec{S}_i^2$ in the eigenstates of \vec{S}_{tot}^2 . Since $\sum_i \vec{S}_i^2$ also commutes with the components of \vec{S}_{tot} , hence with S_{tot}^- and S_{tot}^+ , the expectation value in a state $|S_{\text{tot}}, m\rangle$ does not depend on m , and it is sufficient to calculate it in one member of the family, for instance $|S_{\text{tot}}, m = S_{\text{tot}}\rangle$. The calculation of the expectation value of \vec{S}_i^2 in this state can be done analytically (see Supplemental Material[13]), leading to:

$$\langle \vec{S}_i^2 \rangle_{S_{\text{tot}}} = \frac{2N(N_s - 1)}{N_s^2} + \frac{1}{N_s^2} S_{\text{tot}}(S_{\text{tot}} + 1) \quad (3)$$

As anticipated, $\langle \vec{S}_i^2 \rangle$ is only a function of S_{tot} . This dependence turns out to take the very simple form $S_{\text{tot}}(S_{\text{tot}} + 1)$, but this is by no means a trivial result in the sense that $\sum_i \vec{S}_i^2$ is not simply related to \vec{S}_{tot}^2 . In fact, $\vec{S}_{\text{tot}}^2 = \sum_i \vec{S}_i^2 + \sum_{i \neq j} \vec{S}_i \cdot \vec{S}_j$, and the expectation value of $\vec{S}_i \cdot \vec{S}_j$ in $|S_{\text{tot}}, m = S_{\text{tot}}\rangle$ does not vanish but is given by

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle_{S_{\text{tot}}} = -\frac{2N}{N_s^2} + \frac{1}{N_s^2} S_{\text{tot}}(S_{\text{tot}} + 1) \quad (4)$$

Eq.(3) implies in particular that, in the total singlet, and in the thermodynamic limit $N, N_s \rightarrow +\infty$, $\rho = N/N_s$ fixed, the local value of the square of the spin is given by

$$\langle \vec{S}_i^2 \rangle_{S_{\text{tot}}=0} = 2\rho \quad (5)$$

where ρ is the boson density. Contrary to what one might naively expect, this limiting value is *not* of the form $S(S+1)$ for some integer S . It is however in good agreement with the QMC results obtained for one and two bosons per site [12]. Finally, let us emphasize that, in Eq. (3), S_{tot} can only take even values because it corresponds to the total spin of spin-1 bosons in a single mode, the $\vec{k} = \vec{0}$ one.

Coming back to the Hamiltonian of Eq.(1) in the limit $U_0 = 0, U_2/t \rightarrow 0$, the low-energy spectrum is thus given by

$$E_{S_{\text{tot}}} = -4tN - \frac{N}{N_s} U_2 + \frac{U_2}{2} \frac{1}{N_s} S_{\text{tot}}(S_{\text{tot}} + 1) \quad (6)$$

where the first term is the energy of the non-interacting condensate. The important property is that the slope is proportional to $1/N_s$ and tends to zero in the thermodynamic limit, leading to a quasi-degenerate ground state. In quantum antiferromagnets, this property goes under the name of Anderson's tower of states[14–18]: on the basis of the low-lying states of this tower, it is possible to reconstruct a wave function very close to the Néel state with spins up on one sublattice and down on the other sublattice whose energy is very

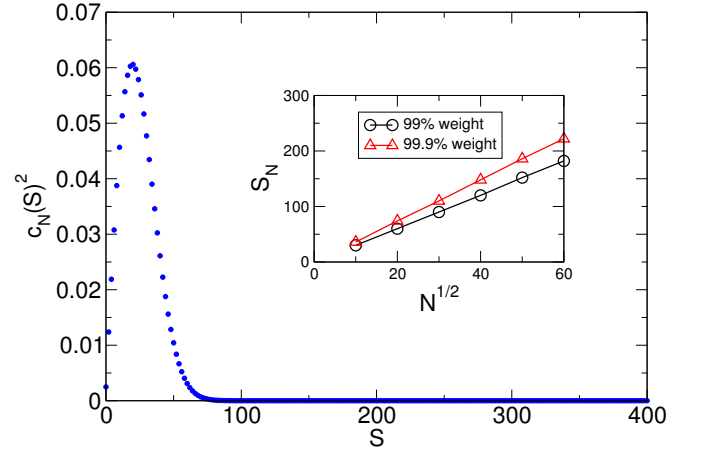


FIG. 1: (Color online) Squares $c_N(S)^2$ of the coefficients of the expansion of the polar state $|\psi_{0,N,0}\rangle$ in the eigenstates $|S, m=0\rangle$ of \vec{S}_{tot}^2 as a function of S for $N = 400$. Inset: value of the spin S_N up to which one has to sum to satisfy the sum rule $\sum_S |c_N(S)|^2 = 1$ to a given accuracy. It scales as \sqrt{N} .

low and scales to the ground state energy when the system size increases, so that the appearance of a tower of states in the low-energy spectrum indicates that the $SU(2)$ symmetry is spontaneously broken in the ground state in favor of antiferromagnetism.

Note that the tower of states remains a well defined concept as long as the energies of the states building this tower are well separated from those of the elementary excitations, which also tend to the ground state energy in ordered systems. In the present calculation, which is performed in the $U_2/t \rightarrow 0$ limit, this is clearly true since the elementary excitations consist in exciting a particle out of the condensate with an energy of order t/N_s for small wave vector, while the states of the tower have energies of order U_2/N_s .

Now, using only states with small values of S_{tot} , it is possible to reconstruct almost exactly polar states. Indeed, all polar states are related by a rotation to $|\psi_{0,N,0}\rangle \propto a_{\vec{k}=\vec{0},0}^{\dagger N} |0\rangle$, and this state can be expanded in the basis of eigenstates of \vec{S}_{tot}^2 as

$$|\psi_{0,N,0}\rangle = \sum_{S=0,2,\dots,N} c_N(S) |S, m=0\rangle$$

The coefficients $c_N(S)$ can be determined analytically[13] and are given by

$$c_N(S) = \sqrt{\frac{(2S+1)N!}{(N-S)!!(N+S+1)!!}} \quad (7)$$

These coefficients only take significant values up to $S = O(\sqrt{N})$: as shown in Fig. 1, the maximum value of the spin S_N up to which one has to sum to satisfy the sum rule $\sum_S |c_N(S)|^2 = 1$ to a given accuracy scales as \sqrt{N} . As a consequence, the polar state $|\psi_{0,N,0}\rangle$ has an energy per site

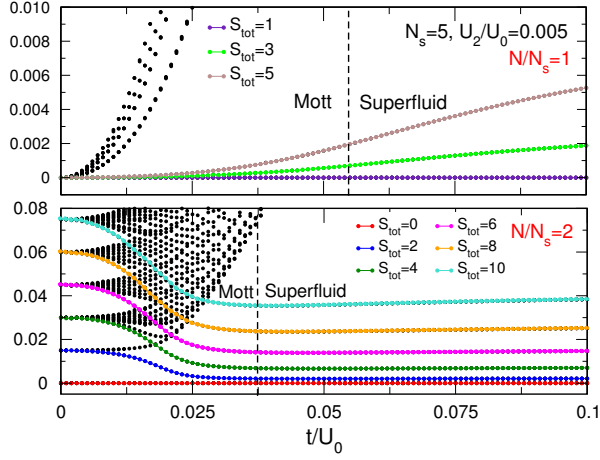


FIG. 2: (Color online) Low energy spectra for 5 sites with $N/N_s = 1$ (up) and $N/N_s = 2$ (bottom) with $U_2/U_0 = 0.005$. The energies are in unit of U_0 and measured from the ground state. The vertical dashed line indicates the Mott-superfluid transition according to the QMC simulations[12].

that scales to the ground state one as $1/N_s$ in the thermodynamic limit. It is thus a ground state in that limit, which proves the presence of long-range nematic order. These results establish that, in the limit $U_0 = 0, U_2/t \rightarrow 0$, the $SU(2)$ symmetry of the superfluid ground state of spin-1 bosons on a lattice is spontaneously broken in favor of nematic order.

It is instructive to compare these results to the case of spin-1 bosons in a trap[19–23]. In the single-mode approximation, the Hamiltonian reads

$$\mathcal{H} = \frac{U_s}{2N} \vec{S}^2 \quad (8)$$

where U_s is the spin interaction energy per atom. The ground state is a non-degenerate singlet with energy $E_0 = 0$, and the excitation energies are given by $E_S = U_s/(2N)S(S+1)$, $S = 2, 4, \dots$. The structure of this spectrum is similar to that of Eq.(6), with in particular a slope that goes to zero as $1/N$ in the thermodynamic limit. Accordingly, the consequences in that limit are very similar: As discussed in Refs.[19–23], spontaneous symmetry breaking takes place since a polar state can be stabilized for infinitesimal quadratic Zeeman coupling in the thermodynamic limit. The decomposition of the polar state into the angular momentum basis also takes a very similar form, our analytical result of Eq.(7) corresponding to the large- q limit of the result of Ref.[23], where the transition between a fragmented condensate and a polar state induced by a quadratic Zeeman coupling q has been investigated in detail.

Let us now turn to the general case. The phase diagram has been previously studied using mean-field theory [8, 24, 25], variational Monte Carlo method [26] and quantum Monte Carlo simulations [12, 27], and some exact results have been established[28]. These methods have led to the conclusion that, for integer filling, there is a superfluid-insulator Mott

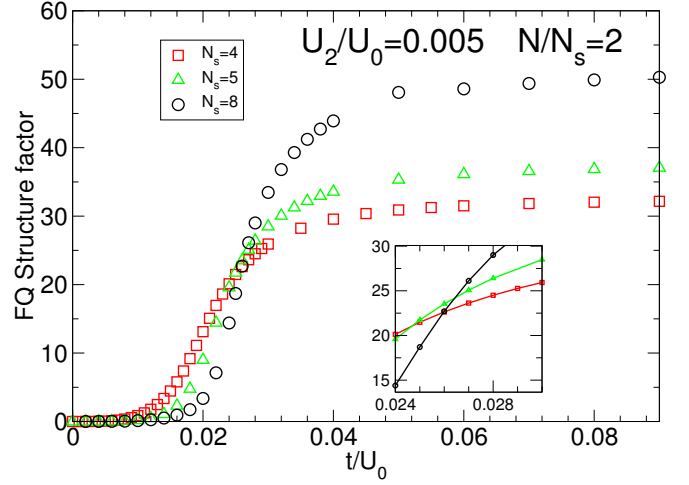


FIG. 3: (Color online) Ferromagnetic quadrupolar structure factor for 4, 5 and 8-site clusters with two bosons per site.

transition upon increasing U_0/t , and the insulating state is always nematic for odd filling while there is an additional nematic-singlet transition upon further increasing U_0/t for even filling. Now that we have analytically demonstrated that the superfluid state is nematic in the limit $U_0/t = 0$ on the basis of the structure of the low-energy spectrum, it is natural to ask to which extent this structure persists away from that limit. For that purpose, we have performed exact diagonalizations of finite-size clusters for one and two bosons per site, with up to 10 and 8 sites respectively. The low energy spectra for 5 sites are depicted in Fig. 2 as a function of t/U_0 . In both cases, the total spin S_{tot} changes by 2 from one state to the next, and the energy of a state measured from the ground state is proportional to $S_{\text{tot}}(S_{\text{tot}} + 1)$, with a coefficient that tends to $U_2/2N_s$ in the large t/U_0 limit, in agreement with Eq.(6). This structure persists below the superfluid-insulator transition without any hint that the system undergoes a phase transition. This suggests that the nematic order predicted previously in the insulating phases is continuously related to the nematic order we have established in the $U_0 = 0, U_2/t \rightarrow 0$ limit. Upon further reducing the ratio t/U_0 , the structure of the tower of states remains essentially unaffected for one boson per site, but a series of level crossings leads to a completely different spectrum for two bosons per site which signals a nematic-singlet transition. The same structure has been observed on larger clusters[13].

In the Mott-insulating phase, the identification of the order as nematic, and *not* antiferromagnetic, actually deserves special attention since, for antiferromagnetic coupled spins, one might in general expect simple Néel order on a bipartite lattice. In exact diagonalizations, antiferromagnetic and nematic order can be distinguished by the quantum numbers that appear in the tower of states. For Néel order, all values of S_{tot} are represented in the tower of states because, to reconstruct the Néel state with up spins on one sublattice and down spins

on the other one, one needs states with both even and odd total spin whereas, for quadrupolar order, one only needs states with even total spin[29, 30]. In view of the analytical results of the $U_0 = 0, U_2/t \rightarrow 0$ limit, we expect by continuity the low-lying states calculated by exact diagonalizations away from that limit to carry only total spin. We have explicitly checked this to be the case for the 5 site cluster. So the fact that only even steps in S_{tot} appear in the tower of states is an additional confirmation that, in the regions of the Mott insulating phases with spontaneously broken SU(2) symmetry the order is indeed nematic.

As an independent confirmation, we have calculated the ferroquadrupolar structure factor $S^Q(\vec{k} = \vec{0})$, with $S^Q(\vec{k}) = \sum_j \exp(i\vec{k} \cdot \vec{r}_j) \langle \vec{Q}_0 \cdot \vec{Q}_j \rangle$, where the quadrupolar operator is defined by $\vec{Q} = [(S^x)^2 - (S^y)^2, 1/\sqrt{3}(2(S^z)^2 - (S^x)^2 - (S^y)^2), S^x S^y + S^y S^x, S^y S^z + S^z S^y, S^z S^x + S^x S^z]$. For two bosons per site, as can be seen in Fig. 3, it increases with the size for large enough t/U_0 , and it decreases with the size for small enough t/U_0 . The crossing point can be taken as an approximation of the transition to nematic order[13], and the critical value $t_c/U_0 \sim 0.026$ is in excellent agreement with the QMC estimate based on the development of a local quadrupolar moment.

In principle, it is possible to locate the singlet-nematic transition just by investigating the spin gap, which is expected to be finite in the singlet phase and to scale to zero in the nematic phase. It turns out that this is not very accurate for the sizes accessible with exact diagonalizations, and only a very rough estimate of the transition can be obtained along these lines[13]. This estimation however is still consistent with other estimates.

Finally, we have attempted to locate the superfluid-insulator transition, which, as usual, corresponds to the opening of the charge gap defined by $\Delta_c = E(N+1) + E(N-1) - 2E(N)$. As for the singlet-triplet gap, the results are consistent with the QMC estimate ($t_c/U_0 \simeq 0.037$), but the sizes accessible to exact diagonalizations do not lead to a very precise estimate. It is only thanks to QMC calculations, with SGF algorithm [31], of the energies for larger system sizes that this criterion can be shown to coincide with the appearance of a superfluid stiffness[12] (see Fig. 4). Note that, for $U_2/U_0 = 0.005$, the superfluid-Mott insulator transition is well separated from the singlet-nematic transition. Increasing U_2 pushes the singlet-nematic transition to larger critical value, and when $U_2/U_0 \sim 0.1$, there is only one transition from the singlet Mott phase to the nematic superfluid left[13].

To summarize, let us put the present results in perspective. Except in one dimension, where Density Matrix Renormalization Group can be used[10, 32, 33], the investigation of lattice bosonic models is largely dominated by QMC, and rightly so since, due to the absence of minus sign problem in many cases, extremely accurate results can be obtained on very large system sizes. Yet, as demonstrated in the present Letter, investigating the excitation spectrum of the model with analytical tools if possible, or with exact diagonalizations of small clus-

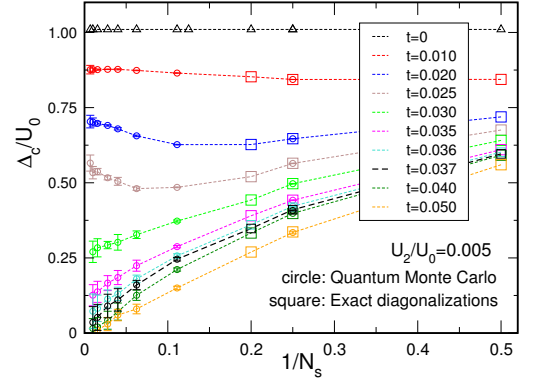


FIG. 4: (Color online) Charge gap as a function of the inverse number of sites for various values of t/U_0 . It opens at $t_c/U_0 \simeq 0.037$, which marks the superfluid-insulator transition.

ters, can lead to very interesting insight into the properties of the system, even if the sizes accessible are much smaller than with QMC. In the present case, the structure of the low-energy spectrum, which consists of an Anderson tower of state in a large portion of the phase diagram, is an extremely fruitful piece of information. In particular, it has led to the demonstration that, in the superfluid phase of spin-1 bosons on a lattice, the SU(2) symmetry is spontaneously broken, by contrast to the case of bosons in a single mode, which require an SU(2) symmetry-breaking interaction to build a polar condensate. It will be very interesting to investigate the implications of this result on the dynamics of spinor condensates[34] in the presence of a lattice.

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Supplemental Material: Anderson tower of states and nematic order of spin-1 bosonic atoms on a 2D lattice

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ANALYTICAL INVESTIGATION OF THE TOWER OF STATES IN THE LIMIT $U_0 = 0, U_2/t \rightarrow 0$.

In this section, we derive the expression given in the main text for the coefficients $c_N(S)$ of the expansion of the polar state and the expectation value of \vec{S}_i^2 in the low-energy states of the Hamiltonian

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} (a_{i,\sigma}^\dagger a_{j,\sigma} + \text{H.c.}) + \frac{U_0}{2} \sum_i n_i(n_i - 1) + \frac{U_2}{2} \sum_i (\vec{S}_i^2 - 2n_i) \quad (1)$$

in the limit $U_0 = 0, U_2/t \rightarrow 0$.

To simplify notations, we introduce an integer n related to S_{tot} by

$$S_{\text{tot}} = N - n$$

where N is the number of bosons, and we define

$$|N - n\rangle \equiv |S_{\text{tot}}, m = S_{\text{tot}}\rangle$$

In addition, since the ground state manifold is only built out of states of zero momentum, we drop the zero momentum from the Fourier transforms and define

$$a_\sigma^\dagger \equiv a_{\vec{k}=\vec{0}, \sigma}^\dagger = \frac{1}{\sqrt{N_s}} \sum_{i=1}^{N_s} a_{i,\sigma}^\dagger$$

where N_s is the number of sites.

With the help of the singlet creation operator $a_0^{\dagger 2} - 2a_{-1}^\dagger a_1^\dagger$, it is clear that $|N - n\rangle$ is of the form:

$$|N - n\rangle \propto a_1^{\dagger(N-n)} (a_0^{\dagger 2} - 2a_{-1}^\dagger a_1^\dagger)^{n/2} |0\rangle$$

In the following, we will need the explicit form obtained after expanding $(a_0^{\dagger 2} - 2a_{-1}^\dagger a_1^\dagger)^{n/2}$. It is given by

$$|N - n\rangle = \frac{1}{\sqrt{\text{Norm}}} \sum_{p=0}^{n/2} (-2)^p \binom{n/2}{p} a_{-1}^\dagger a_0^{\dagger(n-2p)} a_1^{\dagger(N-n+p)} |0\rangle$$

with

$$\begin{aligned} \text{Norm} &= \sum_{p=0}^{n/2} 2^{2p} \binom{n/2}{p}^2 p!(n-2p)!(N-n+p)! \\ &= \frac{n!! (N-n)! (2N-n+1)!!}{(2N-2n+1)!!} \end{aligned}$$

Calculation of $c_N(S)$

In this section, we show how to expand the polar state

$$|\psi_{0,N,0}\rangle \equiv \frac{1}{\sqrt{N!}} a_0^{\dagger N} |0\rangle$$

into the basis of the eigenstates of \vec{S}_{tot}^2 and S_{tot}^z . Since $\langle \psi_{0,N,0} | S_{\text{tot}}^z | \psi_{0,N,0} \rangle = 0$, one can write

$$|\psi_{0,N,0}\rangle = \sum_{S=0,2,\dots,N} c_N(S) |S, m=0\rangle$$

The coefficients $c_N(S)$ are given by

$$c_N(S) = \langle \psi_{0,N,0} | S, m=0 \rangle$$

Now, the state $|S, m=0\rangle$ can be obtained from the state $|S, m=S\rangle$ by applying the S -th power of the lowering operator S^- :

$$|S, m=0\rangle = \frac{S^{(-S)}}{\prod_{p=1}^S \sqrt{S(S+1) - p(p-1)}} |S, m=S\rangle$$

or, using the notations introduced in the previous section $S = N - n$ and $|N - n\rangle = |S, m=S\rangle$,

$$|S = N - n, m=0\rangle = \frac{S^{-(N-n)}}{\prod_{p=1}^{N-n} \sqrt{(N-n)(N-n+1) - p(p-1)}} |N - n\rangle$$

To calculate $c_N(S)$, we only need to know the coefficient of $a_0^{\dagger N} |0\rangle$ in $|S = N - n, m=0\rangle$. Since

$$|N - n\rangle = \frac{1}{\sqrt{\text{Norm}}} \sum_{p=0}^{n/2} (-2)^p \binom{n/2}{p} a_{-1}^\dagger a_0^{\dagger(n-2p)} a_1^{\dagger(N-n+p)} |0\rangle$$

it is clear that the only term that will give a contribution proportional to $a_0^{\dagger N} |0\rangle$ when acting on this state with $S^{-(N-n)}$ is the $p=0$ one, so that

$$\begin{aligned} \langle \psi_{0,N,0} | S^{-(N-n)} | N - n \rangle &= \\ \langle \psi_{0,N,0} | S^{-(N-n)} \frac{1}{\sqrt{\text{Norm}}} a_0^{\dagger n} a_1^{\dagger(N-n)} | 0 \rangle & \end{aligned}$$

Now, in $S^{-(N-n)} \frac{1}{\sqrt{\text{Norm}}} a_0^{\dagger n} a_1^{\dagger(N-n)} | 0 \rangle$, the only term of $S^{-(N-n)}$ that gives a contribution proportional to $a_0^{\dagger N} | 0 \rangle$ is $(\sqrt{2})^{N-n} (a_0^\dagger a_1) ^{N-n}$, and

$$(a_0^\dagger a_1)^{N-n} a_0^{\dagger n} a_1^{\dagger(N-n)} | 0 \rangle = (N-n)! a_0^{\dagger N} | 0 \rangle$$

The scalar product $\langle \psi_{0,N,0} | S, m = 0 \rangle$ can now be simply evaluated, leading to

$$c_N(S) = \frac{(\sqrt{2})^{N-n} \sqrt{N!} (N-n)!}{\sqrt{\text{Norm}} \prod_{p=1}^{N-n} \sqrt{(N-n)(N-n+1) - p(p-1)}}$$

or, in terms of S rather than $N-n$,

$$c_N(S) = \frac{2^{S/2} \sqrt{N!} S!}{\sqrt{\text{Norm}} \prod_{p=1}^S \sqrt{S(S+1) - p(p-1)}}$$

with

$$\text{Norm} = \frac{(N-S)!! S! (N+S+1)!!}{(2S+1)!!}$$

Finally, one can calculate the product that enters $C_N(S)$:

$$\prod_{p=1}^S (S(S+1) - p(p-1)) = (2S)!$$

leading, after some simplifications, to the following explicit expression for the coefficients $c_N(S)$:

$$c_N(S) = \sqrt{\frac{(2S+1) N!}{(N-S)!! (N+S+1)!!}}$$

Calculation of $\langle \vec{S}_i^2 \rangle$

In terms of bosonic operators, the components of the spin operators can be written as $S_i^\alpha = a_{i,\sigma}^\dagger S_{\sigma,\tau}^\alpha a_{i,\tau}$, where $S^\alpha, \alpha = x, y, z$ are the spin-1 matrices, and with implicit summation over repeated spin indices. Then, introducing the Fourier transform $a_{\vec{k},\sigma}^\dagger = (1/\sqrt{N_s}) \sum_{i=1}^{N_s} e^{i\vec{k} \cdot \vec{R}_i} a_{i,\sigma}^\dagger$, one can write

$$\sum_i S_i^\alpha = \sum_{\vec{k}} a_{\vec{k},\sigma}^\dagger S_{\sigma,\tau}^\alpha a_{\vec{k},\tau}$$

$$(\sum_i \vec{S}_i)^2 = \sum_{\vec{k}, \vec{q}} S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha a_{\vec{k},\sigma}^\dagger a_{\vec{k}',\sigma} a_{\vec{q},\mu}^\dagger a_{\vec{q},\nu}$$

$$\sum_i (\vec{S}_i)^2 = \frac{1}{N_s} \sum_{\vec{k}, \vec{k}', \vec{q}} S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha a_{\vec{k},\sigma}^\dagger a_{\vec{k}',\sigma} a_{\vec{q},\mu}^\dagger a_{\vec{k}-\vec{k}'-\vec{q},\nu}$$

Now, since $a_{\vec{k},\sigma} |N-n\rangle = 0$ except when $\vec{k} = \vec{0}$, we get:

$$\begin{aligned} \langle (\sum_i \vec{S}_i)^2 \rangle &= S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha \langle a_{\vec{0},\sigma}^\dagger a_{\vec{0},\sigma} a_{\vec{0},\mu}^\dagger a_{\vec{0},\nu} \rangle \\ &= S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha \langle a_{\vec{0},\sigma}^\dagger [\delta_{\tau,\mu} + a_{\vec{0},\mu}^\dagger a_{\vec{0},\tau}] a_{\vec{0},\nu} \rangle \\ &= 2N + S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha \langle a_{\vec{0},\sigma}^\dagger a_{\vec{0},\sigma} a_{\vec{0},\mu}^\dagger a_{\vec{0},\mu} \rangle \quad (2) \end{aligned}$$

where all expectation values are taken in the state $|N-n\rangle$, and where we have used the identity $S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha \delta_{\tau,\mu} = (\vec{S}^2)_{\sigma,\nu} = 2\delta_{\sigma,\nu}$. Similarly,

$$\begin{aligned} N_s \langle \sum_i (\vec{S}_i)^2 \rangle &= \sum_{\vec{q}} S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha \langle a_{\vec{0},\sigma}^\dagger a_{\vec{q},\tau} a_{\vec{q},\mu}^\dagger a_{\vec{0},\nu} \rangle \\ &= \sum_{\vec{q}} S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha \langle a_{\vec{0},\sigma}^\dagger [\delta_{\tau,\mu} + a_{\vec{q},\mu}^\dagger a_{\vec{q},\tau}] a_{\vec{0},\nu} \rangle \\ &= 2N_s N + S_{\sigma,\tau}^\alpha S_{\mu,\nu}^\alpha \langle a_{\vec{0},\sigma}^\dagger a_{\vec{0},\sigma} a_{\vec{0},\mu}^\dagger a_{\vec{0},\mu} \rangle \quad (3) \end{aligned}$$

Comparing Eqs. (2) and (3), we get:

$$N_s \langle \sum_i (\vec{S}_i)^2 \rangle = \langle (\sum_i \vec{S}_i)^2 \rangle + 2N(N_s - 1)$$

which, since $\langle (\vec{S}_i)^2 \rangle$ is independent of i , and since $\langle (\sum_i \vec{S}_i)^2 \rangle = S_{\text{tot}}(S_{\text{tot}} + 1)$, leads to

$$\langle \vec{S}_i^2 \rangle = \frac{2N(N_s - 1)}{N_s^2} + \frac{1}{N_s^2} S_{\text{tot}}(S_{\text{tot}} + 1)$$

EXACT DIAGONALIZATION OF THE SPIN-1 BOSON MODEL

Method and clusters

We have numerically studied the spin-1 boson model on small square clusters by exact diagonalizations. For two bosons per site, we could study clusters with $N_s = 2, 4, 5$ and 8 sites. For one boson per site, an additional cluster with $N_s = 10$ has also been studied. The clusters with $N_s = 5, 8, 10$ are depicted in Fig. 1. The most numerical demanding task was the case with 16 spin-1 bosons on the 8-site cluster. The $S_z = 0$ sector is of dimension 3 567 373 818. We have used the hash function for bosons from Ref.[1], and we have used the “sublattice coding” trick [2] for fast searching.

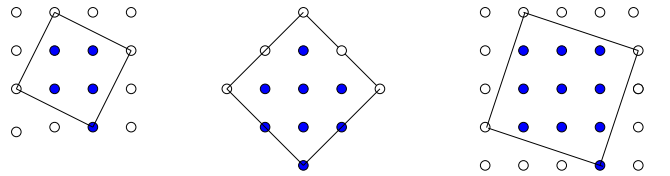


FIG. 1: (Color online) Sketches of the square clusters with $N_s = 5, 8$ and 10.

Tower of states

The two largest calculations are shown in Fig. 2. In both cases, one can clearly see the structure of the tower states. Here we only show spectrum in the $\vec{k} = (0, 0)$ sector for clarity since other momenta do not enter the low energy spectrum

in the nematic phases. For $N_s = 10$ and one boson per site, we can always resolve the five low energy excitations for all nonzero t/U_0 . For two bosons per site and $N_s = 8$, eight excitations can be clearly identified from large to intermediate values of t/U_0 until a series of level crossing takes place.

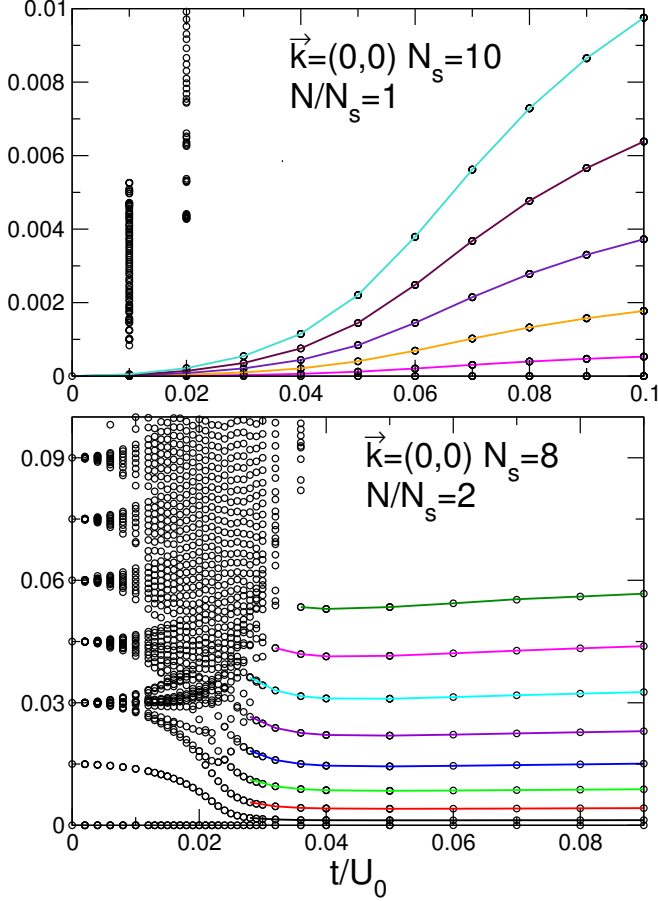


FIG. 2: (Color online) Low energy spectra in $\vec{k} = (0, 0)$ sector for 10 sites with $N/N_s = 1$ and 8 sites with $N/N_s = 2$. Both calculations are done for $U_2/U_0 = 0.005$.

To check the scaling of these low energy excitations with $S(S+1)$, we have plotted their energy as a function of $S(S+1)$ for several values of t/U_0 in Fig. 3. As expected, these curves are nearly perfectly linear. Note however that the dependence of the slope on the ratio t/U_0 is quite different in both cases. For one boson per site, the slope goes to zero because all states are continuously connected to the ground state manifold in the $t/U_0 \rightarrow 0$ limit, while for two bosons per site the slope does not change much, a consequence of the fact that the various states are connected to states with different numbers of spin-2 sites in the $t/U_0 \rightarrow 0$ limit.

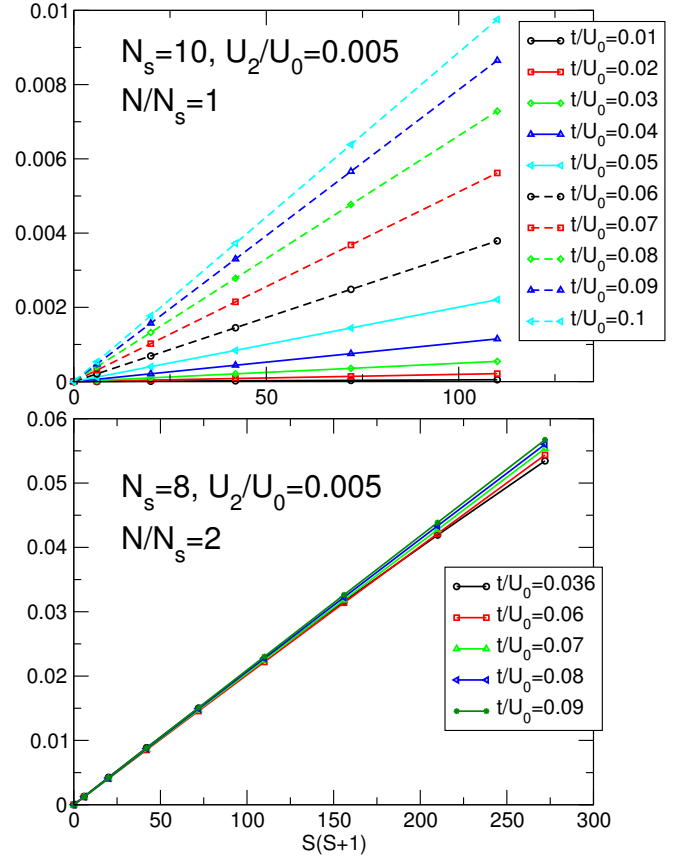


FIG. 3: (Color online) Plot of the low-lying excitations as a function of $S(S+1)$. The expected linear scaling is manifest.

Analysis of the level crossings

The series of level crossing signals a phase transition and can be used to estimate the critical point. In the singlet phase the system is expected to have a gap due to the U_2 term while the nematic phase is gapless. Thus we have tracked the level crossings from the singlet phase, and we have determined the location of the first and second level crossings for different sizes as shown in Fig. 4. We do not have any precise analytical prediction for the scaling of these level crossings, but their evolution with the system size is consistent with the QMC prediction based on the development of a local quadrupole.

Ferroquadrupolar structure factor

To get an alternative indication of the presence of long-range nematic order, we have studied the ferroquadrupolar structure factor (see main text). The scaling of the structure factor with the number of sites N_s is shown in Fig. 5. It increases linearly with the system size for large enough t/U_0 , which indicates that there is indeed nematic long-range order. For $t/U_0 \leq 0.026$, by contrast, the structure factor decreases with the number of sites, which is clearly inconsistent with ne-

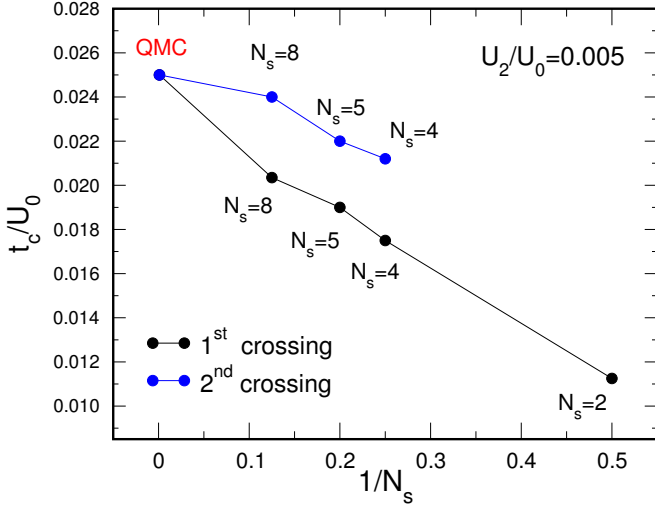


FIG. 4: (Color online) Finite-size analysis of the first two level crossings for the $N/N_s = 2$ case. Their location is consistent with the QMC estimate.

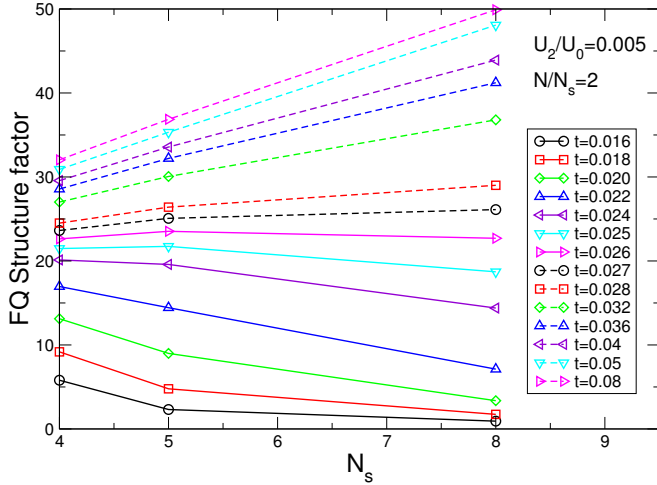


FIG. 5: (Color online) Scaling of the ferroquadrupolar structure factor with the number of sites N_s for various values of t/U_0 .

matic long-range order. To get a precise estimate of the transition, one should be able to identify the point below which the structure factor does not diverge any more, which would require to be able to reach much larger system sizes than available to exact diagonalizations. However, it is plausible that the transition takes place at the point where the structure factor starts to decrease with the size, i.e. between $t/U_0 = 0.026$ and $t/U_0 = 0.027$, again in agreement with the QMC prediction based on the development of a local quadrupole. This change of behavior appears as a level crossing in the figure of the main text.

Spin gap

Another way to estimate the critical value of t/U_0 between the singlet and nematic phases is to calculate spin gaps. In-

deed, in the nematic phase, the gap to spin-2 excitations $\Delta_{S=2}$ (the singlet-quintuplet gap) vanishes, while in the singlet phase all gaps remain finite. The dependence of $\Delta_{S=2}$ with the size of the clusters is shown in Fig.6 for $U_2/U_0 = 0.005$. There is a clear change of behavior for $t/U_0 \leq 0.026$, in reasonable agreement with other estimates. However, to be able to determine the precise value to t/U_0 below which the gap vanishes, one should have access to larger sizes.

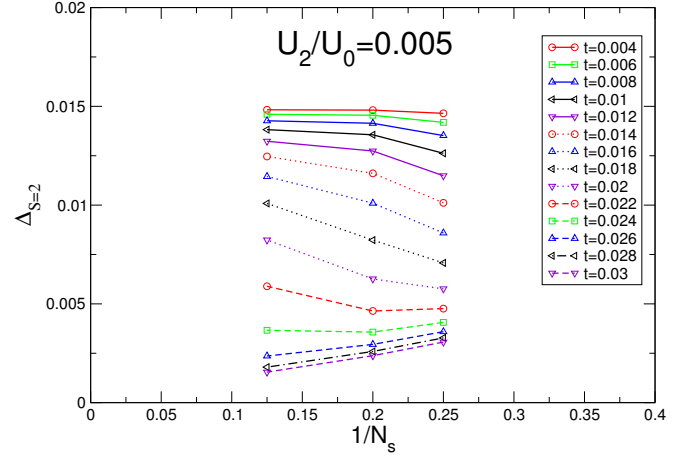


FIG. 6: (Color online) Scaling of the gap to spin-2 excitations with the number of sites N_s for various values of t/U_0 .

Dependence of the singlet-to-nematic transition on U_2

We have also studied the ferroquadrupolar structure factor for other values of U_2/U_0 (see Fig.7). The critical values t_c/U_0 derived from this analysis match those estimated by QMC in Ref.[3] very well. For larger values of U_2/U_0 the nematic region inside Mott phase decreases, and for $U_2/U_0 = 0.1$ it seems that the singlet-to-nematic transition coincides with the Mott-superfluid transition.

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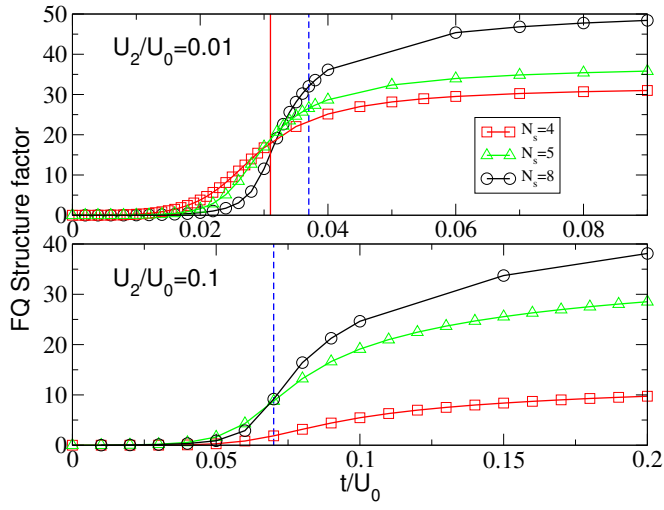


FIG. 7: (Color online) Ferroquadrupolar structure factor for two bosons per site for clusters with $N_s = 4, 5$, and 8 sites. The vertical dashed (blue) lines indicate the Mott insulator to superfluid transition taken from Ref.[3] and the vertical straight (red) line indicates the transition between the singlet and nematic phases.